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Artificial Neural Network Regression-based Modelling of a Charging Solid State Hydrogen Compression Unit

Douw G Faurie, Kasturie Premlall and Andrei Kolesnikov
Department of Chemical, Metallurgical, and Materials Engineering
Tshwane University of Technology
Pretoria, Republic of South Africa
GerbrandFaurie@gmail.com, PremlallK@tut.ac.za, KolesnikovA@tut.ac.za

Mykhaylo Lototskyy
HySA Systems, South African Institute for Advanced Materials Chemistry
University of the Western Cape
Cape Town, Republic of South Africa
MLototskyy@uwc.ac.za

Abstract

With hydrogen as a clean but hazardous energy carrier, solid-state hydrogen storage in the form of a metal hydride has come forth as a safe and low-pressure storage solution with competitive volumetric energy density. This paper reports the modelling of a metal hydride reactor during its charge state using neural network regression. This was done by generating a validated finite element model of the reactor, which was then used to generate dynamic operational data based on the feed pressure and cooling fluid temperature as independent variables. The best-performing neural network model validation using the experimentally observed data achieved a regression coefficient of 0.99 and a mean squared error of around 10-4. This predictive model, with further refinement, can be implemented to allow predictive control, which has always been a challenge through conventional means due to the batch nature of the system. Moreover, the hydrogen concentration as stored in a solid-state measurement would be too expensive for industrial applications.

Keywords
Metal Hydride Reactors, Artificial Neural Networks (ANNs), Hydrogen Desorption, Hydrogen Absorption

1. Introduction
Solid-state hydrogen storage refers to the storage of hydrogen in a solid form, in particular, through bulk absorption to form metal hydrides. These metal hydrides are created through a reaction that requires cooling and decompose during heating to release the stored hydrogen. This technology partially addresses the challenges associated with liquid and gas phase storage. (Yartys & Lototsky, 2004; Churchard et al., 2011; Prachi, Wagh & Aneesh, 2016; Krane et al., 2022; Adhy Lesmana et al., 2024). Furthermore, solid-state hydrogen storage has a very limited environmental impact, as reported by Costamagna et al. (Costamagna et al., 2022).

This can be seen in studies by Baldissin et al., Peng et al., and Chibani et al. (2009; Chibani et al., 2024; Peng et al., 2024), the implementation of the finned heat sinks in a hydride reactor led to superior cooling compared to a reactor that did not have a heat transfer-aided design. Generally, the design of the metal hydride reactor is based on the heat transfer enhancement of the bed. As such, two common variants exist: firstly, with heat transfer from the outside and secondly, with heat transfer from the inside (Lototskyy et al., 2017; Dong et al., 2022; Aadhithiyan & Anbarasu, 2024).

A comprehensive literature review on metal hydride reactor design was published by Cui et al. (Cui et al., 2022) considered heat-sink and various internal cooling designs. Specifically, internal configurations of radial tubes, helical tubes and straight pipe heat exchangers were considered and compared. However, there is a clear lack of analysis on a design using both a cooling jacket and internal cooling. Similarly, there is a clear knowledge gap in the effects of scaling reactors in diameter with internal cooling setups.

Additionally, the studies reviewed by Cui et al. (Cui et al., 2022) did not consider the trade-off of consuming some of the overall reactor volumes with heat exchangers, lowering the effective bed volume and ultimately the capacity of the reactor. Lui et al. (Liu et al., 2014) did report the effects of tube pitch of internal straight pipe heat exchangers, though for only a singular pipe size, and there has not been a significant contribution to the knowledge gap since.

Conventional control systems require a feedback approach which measures responses and adjusts accordingly. Alternatively, control systems require predictive control, which needs to be able to predict changes in the response parameters with changes in input parameters. Solid-state hydrogen storage poses a unique challenge for control systems, being a complex batch system with changes being felt with a long delay after changes have been made. This is compounded by the cost of sensors that can measure hydrogen concentration stored in a solid state, which are too expensive to be economically feasible. Thus, the ability to design an effective control system around a metal hydride-based hydrogen storage system requires a predictive model to be referenced by the control system (Verma et al., 2025).

2. Method

Experimental equipment and experimental data to validate this study were supplied by HySA-Systems under the umbrella of the University of the Western Cape (Lototskyy et al., 2018). Figure 1 represents a schematic diagram of the experimental setup filled with $LaNi_{4.9}Sn_{0.1}$ hydride-forming metal. This unit is an industrial unit, used to compress hydrogen, installed at a mine in the Northwest. Thus, tests were then performed at normal operational conditions so as not to disrupt the operation of the mine. For the charging validation data, the feed gas pressure delivered to the unit was set at 5.5 bar and 4.9 bar on the regulator, and to cool the reactor, water at 15 °C and 18 °C was used.

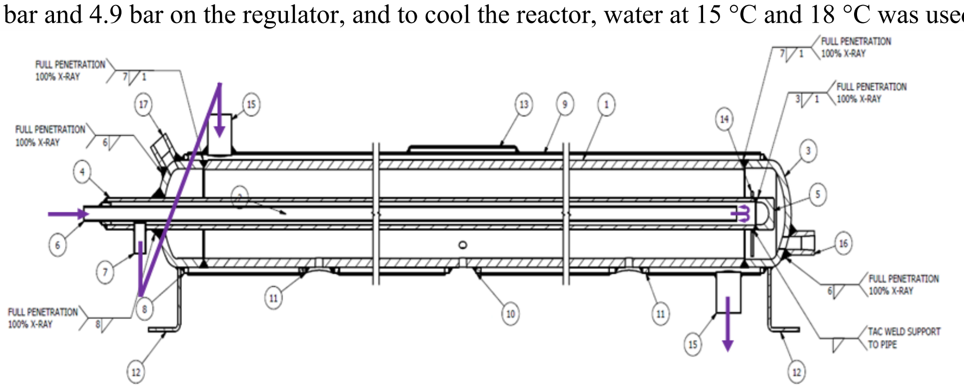

Figure 1. Schematic diagram of a hydride-based hydrogen compressor

For the finite element model, the method reported by Faurie et al. (2025) was implemented. COMSOL Multiphysics was used with an ideal gas assumption. Considering the bed expansion, the assumption was made that 25% volumetric expansion is linearly proportional to concentration. To avoid large temperature difference computation in the first few minutes of the dynamic simulation, initial temperature and pressure were set to the feed gas pressure and cooling fluid temperature. Finally, gas in bed transport was considered to follow Darcy's law and a porous heat transfer model was used. The flow of the hydrogen gas can be simplified to Darcy's Law to account for the pressure drop over the porous bed, represented by Equations 1 and 2 (Wang et al., 2019).

$$\frac{\partial}{\partial t}\left(\varepsilon_p \rho\right) + \nabla(\rho u) = Q_m \tag{1}$$

$$u = -\frac{K}{\mu}\nabla p \tag{2}$$

Likewise, the flow of heat in the porous bed can be simplified to a porous heat conduction law, which combines convective and conductive heat transfer, represented by Equations 3 and 4 (Wang et al., 2019).

$$\left(\rho C_p\right)_{eff}\frac{\partial}{\partial t} + \rho C_p u \cdot \nabla T + \nabla q = Q + Q_{vd} \tag{3}$$

$$q = -k_{eff}\nabla T \tag{4}$$

The rate of hydrogen sorption in the metal hydride (Adapted from (Mellouli et al., 2009; Xiao et al., 2017; Dunikov et al., 2021; Jithu & Mohan, 2022; Chibani et al., 2024)) represented by equation 5.

$$\dot{m} = C_A exp\left(-\frac{E_A}{RT}\right) ln\left(\frac{P_g}{P_{eq}}\right)(\rho_{ss} - \rho_s) \tag{5}$$

To solve the equilibrium pressure, the computational methodology laid out by Faurie & Permlall (2025) was implemented. Along with the fitting parameters reported by Faurie & Premlall (2025) using the script reported by Faurie et al (2025). The parameter tables of the simulation were used, as reported by Faurie et al. (2025). The boundary assumptions are that the ends are thermally isolated, and the reactor is heated through the inner and outer heat exchanger surfaces. Hydrogen is only fed through one end of the tank, and the other end is set as a dead end for hydrogen.

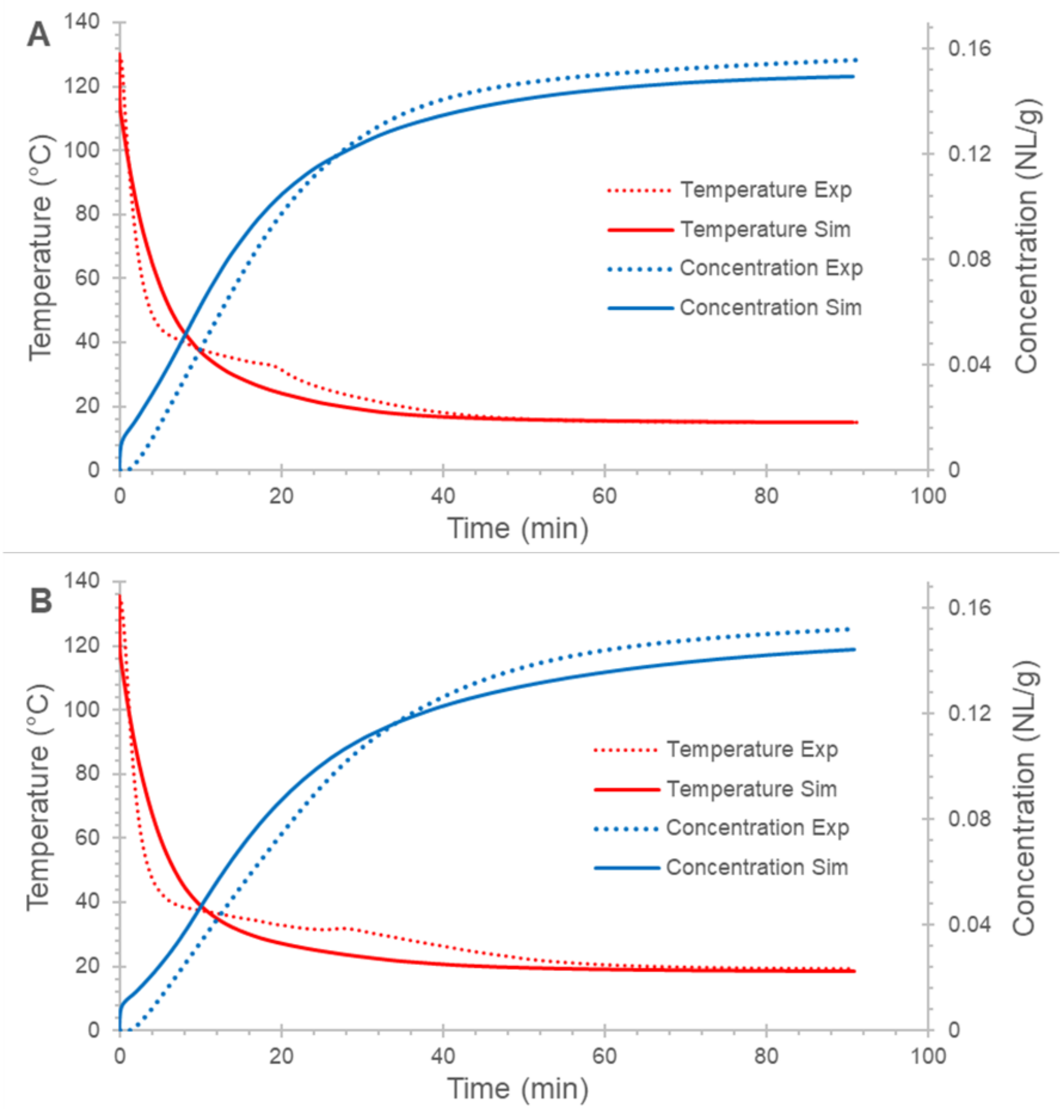

Figure 2. Computational fluid dynamics validation with time versus concentration and temperature with (A) feed gas pressure at 5.5 bar with cooling fluid at 15 °C and (B) feed gas pressure at 4.9 bar with cooling fluid at 18 °C

Figure 2 shows the performance of the model. This model was then used to generate training data by varying the operational input parameters and measuring the dynamic output. This data was then used to train an artificial neural network using the feed gas pressure, cooling fluid temperature, and time as inputs and concentration as the variable the neural network would predict. These neural networks would vary in layer count and hidden neuron count using a ReLU activation and the Levenberg-Marquardt training algorithm. For this, both MathWorks MATLAB and TensorFlow were used with a 70-15-15 Training-Testing-Validation split. The trained models would then be re-validated against the experimental data, and performance would be analysed in terms of R-squared and mean-squared-error, which can be considered measures of precision and accuracy of the model. Using simulated data to train the neural networks bypassed the need for extensive and expensive experimental trials.

3. Results and Discussion

Figure 3 shows the final mean squared error of the nine different neural network architectures when evaluated on the experimental data regarding the charge state. This is a fully connected neural network with one to three hidden layers and 5, 10, or 20 neurons on each hidden layer. The mean squared error units on the y-axis have been adjusted for ease of understanding. Thus, the true recorded value is the number indicated by the y-axis x10-4 as indicated on the top left of the y-axis. Regarding Figure 3, the single-layer network architecture has a stable mean squared error regardless of the number of neurons in the hidden layer. While the multi-layered network architectures all have less desirable performance as the number of neurons in the hidden layers increases. However, further assessment is needed because a lower mean squared error can be an indication of overfitting.

Figure 4 represents the R-squared performance of the nine neural network architectures when tested on the experimental data regarding the charge state. This R-squared is observed during the linear regression of model-predicted values and the experimentally observed values. During this application, this may be referred to as the adjusted R-squared statistic, as it does not measure the fit of the model on the dynamic data but only considers the predicted and observed data. This R-squared statistic measures how closely the model-predicted and experimentally observed data reflect each other; thus, a value closer to one is desired. Regarding Figure 4, it can be observed that only the single-layer network architecture performed desirably regardless of the number of neurons.

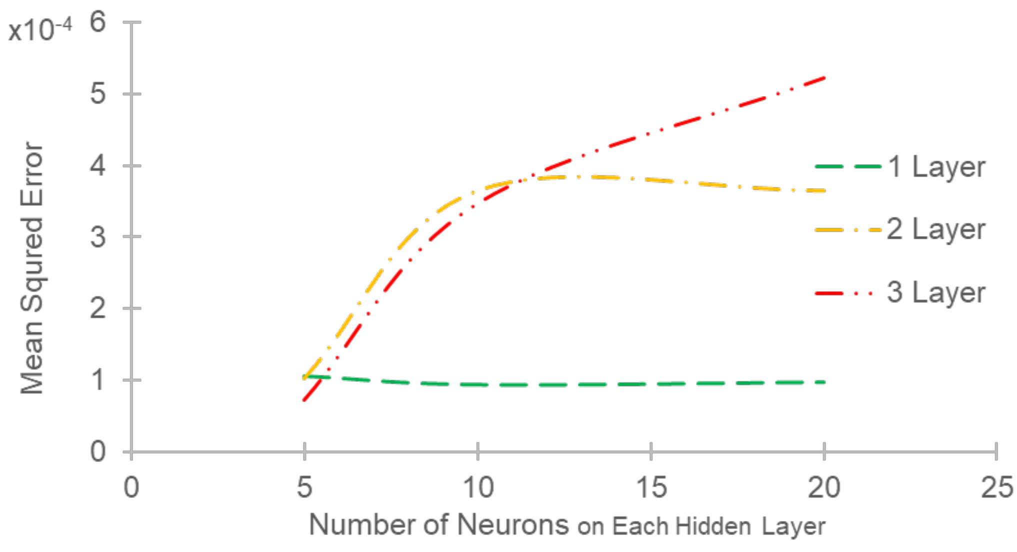

Figure 3. Absorption mean-squared error performance of the different neural network architectures when tested on the experimental data.

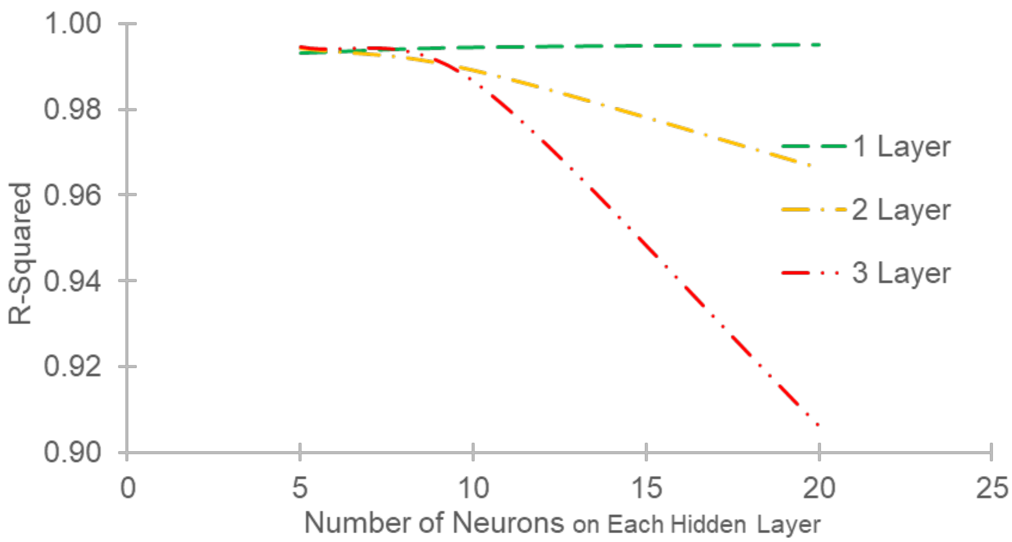

Figure 4. Absorption R-squared performance of the different neural network architectures when tested on the experimental data.

Considering the analysis of Figures 3 and 4, it was determined that the single-hidden-layer neural network with ten neurons on the hidden layer is the best-performing neural network architecture tested. A fair case could be made for the other single hidden layer neural network architectures, but it was determined that the ten neurons on the hidden layer architecture was slightly better performing without over-complexity.

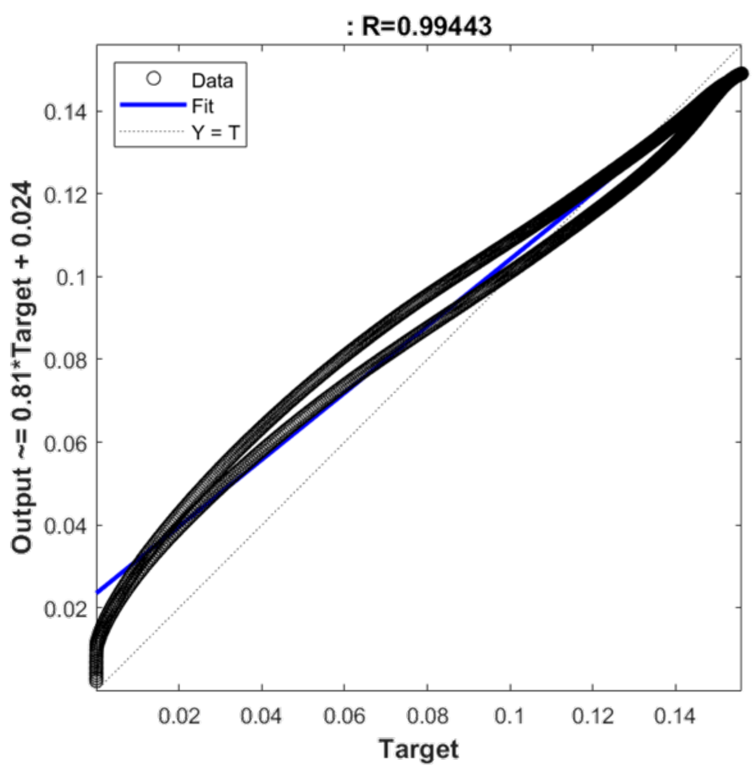

Figure 5. Absorption regression of the single-layer, 10-neuron hidden-layer network architecture model predictions against experimental data.

Figure 5 represents the linear regression of the model-predicted values (Output on the y-axis) against the experimentally observed data (Target on the x-axis) regarding the charge state. Specifically, for the single hidden layer, a ten-neuron-layer neural network architecture was used, which was determined to be the best-performing neural network architecture for absorption. Here, the "Y=T" line represents perfect prediction by the model. The R-squared in this instance was determined to be 0.99443, or rounded to 0.9944.

Regarding Figure 5, the two distinct curves that formed seem to be the two different experimental trials, having differing degrees of accuracy for the whole of the dataset. Furthermore, there is an overshoot from the model in most of the dataset, and then a subsequent undershoot in the rest of the dataset. This is similar to the discharge model, while within the bounds of accuracy, this indicates the model is not perfect. Accuracy can be improved by the availability of more data at varied operational parameters

4. Conclusion

The best-performing artificial neural network model achieved a regression coefficient of 0.99 and a mean squared error of less than 10-4 during training. Likewise, the best-performing neural network model validation using the experimentally observed data achieved a regression coefficient of 0.99 and a mean squared error of less than 10-4. This proves that neural networks can model the complexity of metal hydride reactors during discharge, specifically the HySA-systems Metal Hydride reactor prototype.

This work serves as proof of concept that a predictive digital twin model can be generated for the discharge state of metal hydride reactors with further refinement. This refinement would come in the form of further computational fluid dynamics model validation and increasing the number of permutations of situations that would be used to train the artificial neural network. Such as partial capacity discharge.

Nomenclature

$\dot{m}$	-	Hydrogen sorption rate in mass/volume/time			
ρ_s	-	Dynamic hydride density	ρ_0	-	Standard hydride density
P_g	-	The pressure of the gas in the tank	P_{eq}	-	The pressure of the gas in the hydride
T	-	Temperature	R	-	Ideal gas constant
C_A	-	Adsorption rate constant	E_A	-	Adsorption activation energy

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References

Aadhithiyan, A.K. & Anbarasu, S. Computational fluid modeling of lanthanum-based hydrogen storage reactors for heat pump applications. *International Journal of Heat and Fluid Flow*. 108:109439. 2024.DOI: 10.1016/J.IJHEATFLUIDFLOW.2024.109439.

Adhy Lesmana, L., Lu, C., Chen, F. & Aziz, M. Topology optimization of gyroid structure-based metal hydride reactor for high-performance hydrogen storage. *Thermal Science and Engineering Progress*. 2024. 50:102533. DOI: 10.1016/J.TSEP.2024.102533.

Baldissin, D. & Lombardo, D. Thermofluidynamic Modelling of Hydrogen Absorption and Desorption in a LaNi4.8Al0.2 Hydride Bed. In *Proceedings of the COMSOL Conference*. Milan. 1–7. 2009.

Chibani, A., Boucetta, C., Merouani, S., Tounsi, A., Adjel, S., Lamiri, L., Bouchoul, B. & Merabti, H. Impact of fins and cooling fluid on the hydrogenation process in a LaNi5-Based metal hydride reactor for hydrogen storage. *International Journal of Hydrogen Energy*. 69:134–146. 2024. DOI: 10.1016/J.IJHYDENE.2024.04.314.

Churchard, A.J., Banach, E., Borgschulte, A., Caputo, R., Chen, J.-C., Clary, D., Fijalkowski, K.J., Geerlings, H., et al. A multifaceted approach to hydrogen storage. *Physical Chemistry Chemical Physics*. 13(38):16955. 2011.DOI: 10.1039/c1cp22312g.

Costamagna, M., Barale, J., Carbone, C., Luetto, C., Agostini, A., Baricco, M. & Rizzi, P. Environmental and economic assessment of hydrogen compression with the metal hydride technology. *International Journal of Hydrogen Energy*. 47(17):10122–10136. 2022.DOI: 10.1016/j.ijhydene.2022.01.098.

Dong, Z., Wang, Y., Wu, H., Zhang, X., Sun, Y., Li, Y., Chang, J., He, Z., et al. A design methodology of large-scale metal hydride reactor based on schematization for hydrogen storage. *Journal of Energy Storage*. 49:104047. 2022. DOI: 10.1016/j.est.2022.104047.

Dunikov, D.O., Borzenko, V.I., Blinov, D. V, Kazakov, A.N., Romanov, I.A. & Leontiev, A.I. Heat and mass transfer in a metal hydride reactor: combining experiments and mathematical modelling. *Journal of Physics: Conference Series*. 2057(1):012122. 2021.DOI: 10.1088/1742-6596/2057/1/012122.

Faurie, D.G. & Premlall, K. Simulating non-ideal AB5 metal hydride pressure–concentration–temperature isotherms in MATLAB. *Multiscale and Multidisciplinary Modeling, Experiments and Design*. 8(3):194. 2025.DOI: 10.1007/s41939-025-00780-9.

Faurie, D.G., Premlall, K. & Koech, L.K. High-Resolution Simulated Metal Hydride Pressure-Concentration-Temperature Isotherm Data with Software. *Chemical Data Collections*. preprint:101202. 2025. DOI: 10.2139/ssrn.5260703.

Faurie, D., Premlall, K., Kolesnikov, A. & Lototskyy, M. Sensitivity Analysis of a Metal Hydride Reactor Utilizing LaNi4.9Sn0.1 Metal Hydride. In *Proceedings of the International Conference on Industrial Engineering and Operations Management*. Michigan, USA: IEOM Society International. 2025.DOI: 10.46254/EU08.20250222.

Jithu, P. V. & Mohan, G. Performance simulation of metal hydride based helical spring actuators during hydrogen sorption. *International Journal of Hydrogen Energy*. 47(33):14942–14951. 2022. DOI: 10.1016/j.ijhydene.2022.02.234.

Krane, P., Nash, A.L., Ziviani, D., Braun, J.E., Marconnet, A.M. & Jain, N. Dynamic modeling and control of a two-reactor metal hydride energy storage system. *Applied Energy*. 325:119836. 2022. DOI: 10.1016/j.apenergy.2022.119836.

Liu, Y., Wang, H., Prasad, A.K. & Advani, S.G. Role of heat pipes in improving the hydrogen charging rate in a metal hydride storage tank. *International Journal of Hydrogen Energy*. 39(20):10552–10563. 2014.DOI: 10.1016/J.IJHYDENE.2014.04.197.

Lototskyy, M., Klochko, Y., Wafeeq Davids, M., Pickering, L., Swanepoel, D., Louw, G., van der Westhuizen, B., Chidziva, S., et al. Industrial-scale metal hydride hydrogen compressors developed at the South African Institute for Advanced Materials Chemistry. *Materials Today: Proceedings*. 5(4):10514–10523. 2018.DOI: 10.1016/j.matpr.2017.12.383.

Lototskyy, M. V., Tolj, I., Pickering, L., Sita, C., Barbir, F. & Yartys, V. The use of metal hydrides in fuel cell applications. *Progress in Natural Science: Materials International*. 27(1):3–20. 2017.DOI: 10.1016/j.pnsc.2017.01.008.

Mellouli, S., Askri, F., Dhaou, H., Jemni, A. & Ben Nasrallah, S. Numerical study of heat exchanger effects on charge/discharge times of metal–hydrogen storage vessel. *International Journal of Hydrogen Energy*. 34(7):3005–3017. 2009.: 10.1016/j.ijhydene.2008.12.099.

Peng, C., Liu, X., long, R., Liu, Z. & Liu, W. Performance optimization of adsorption hydrogen storage system via computation fluid dynamics and machine learning. *Chemical Engineering Research and Design*. 207:100–109. 2024.DOI: 10.1016/J.CHERD.2024.05.022.

Prachi, P., Wagh, M.M. & Aneesh, G. A Review on Solid State Hydrogen Storage Material. *Advances in Energy and Power*. 4(2):11–22. 2016.DOI: 10.13189/aep.2016.040202.

Verma, S., Kishore, R.A., Kumar, K. & Mitra, P.R. Dynamic modelling and control strategy of a temperature-driven metal hydride cooling system for buildings. *Energy and Buildings*. 331:115381. 2025.DOI: 10.1016/j.enbuild.2025.115381.

Wang, D., Wang, Y., Huang, Z., Yang, F., Wu, Z., Zheng, L., Wu, L. & Zhang, Z. Design optimization and sensitivity analysis of the radiation mini-channel metal hydride reactor. *Energy*. 173:443–456. . 2019 DOI: 10.1016/J.ENERGY.2019.02.033.

Xiao, J., Tong, L., Yang, T., Bénard, P. & Chahine, R. Lumped parameter simulation of hydrogen storage and purification systems using metal hydrides. *International Journal of Hydrogen Energy*. 42(6):3698–3707. 2017.DOI: 10.1016/j.ijhydene.2016.11.060.

Yartys, V.A. & Lototsky, M. V. An Overview of Hydrogen Storage Methods. In *Hydrogen Materials Science and Chemistry of Metal Hydrides*. V. 172. 75–104. 2004.DOI: 10.1007/1-4020-2669-2_7.

Biographies

Douw Gerbrand Faurie is a Doctor of Engineering graduate in the discipline of Chemical Engineering from the Tshwane University of Technology, scheduled to graduate in 2025. He graduated Master of Engineering in Chemical Engineering Cum Laude in 2022, with his research focusing on improving the design practices and the knowledge base regarding metal hydride-based hydrogen storage tanks using computational fluid dynamics. Currently, Douw serves as a post-doctoral research fellow at the Tshwane University of Technology, investigating composite adsorption nanoparticles.

Dr Kasturie Premlall is a permanently appointed Researcher and Lecturer in the Department of Chemical, Metallurgical and Materials Engineering, Faculty of Engineering and the Built Environment at Tshwane University of Technology, Pretoria, South Africa. She has previously held the position of Section Head for Chemical Engineering. She has completed a Master's degree in corrosion inhibition studies of the degradation of reinforcement steel in structural materials, focusing on reinforcement of concrete structures and ion-metal ingress. She earned her PhD in Chemical Engineering from the University of Witwatersrand, South Africa. Her focused research interests include carbon capture and sequestration (CCS), corrosion technology focusing on green corrosion inhibitors, hydrogen storage and metal-organic frameworks (MOFs) for carbon dioxide (CO2) capture; landfill biogas recovery (process and materials) for methane (CH4) capture and the recovery, and interest in rare earth elements (REEs) from AMD and coal fly ash in South Africa.

Prof Andrei Kolesnikov graduated from the Moscow Institute of Chemical Engineering in 1979. He obtained a PhD degree from the same institution in 1985. The topic of his PhD work was entitled "Multi-jet plasma chemical reactor for aluminium oxide nanopowder production". He worked as an applied researcher in the State Laboratory of Plasma Processes at Almaty Power Engineering Institute from 1979 to 1992. He continued his research work in South Africa, where he worked at the Nuclear Energy Corporation of South Africa from 1992 to 1999, and at Tshwane University of Technology from 1999 up to 2022. His research interests include the modelling of multi-phase high-temperature processes, plasma technologies, agent-based modelling of complex systems, and process control and optimisation.

Dr Mykhaylo Lototskyy graduated from Moscow State University in 1977 and received his PhD degree in 1992 from the Lviv State University (Ukraine). He held postdoctoral positions at the Institute for Energy Technology (Norway, 2002–2003) and the University of the Western Cape. Currently, Dr Lototskyy is a Senior Researcher at the South African Institute for Advanced Materials Chemistry and a Key Technology Specialist on Hydrogen Storage and Related Applications within the South African Hydrogen and Fuel Cell Technologies RDI Program (HySA Systems Competence Centre hosted by UWC). Dr Lototskyy is an internationally recognised and renowned researcher in the fields of Hydrogen Energy and Technology, hydrogen storage, material science and applications of metal hydrides.